Center for Bio-Inspired Energy Science (CBES) EFRC Director: Samuel I. Stupp Lead Institution: Northwestern University

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Mission Statement: To discover and develop bio-inspired systems that reveal new connections between energy and matter.

The goal of the Center for Bio-inspired Energy Science (CBES) is to develop artificial materials and systems that take inspiration from biology to optimize the way we use energy and interconvert between different energy forms, for example converting chemical energy into mechanical energy the way muscles do in living organisms. Our team members have innovated in the areas of self-assembly, the interface of biology and materials science, as well as in theory and simulation. CBES research addresses the following two DOE grand challenges: "how do we characterize and control matter away-especially very far away-from equilibrium?" and "how can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?" Our work also addresses the DOE's basic research need for "new science for a secure and sustainable energy future." CBES is scientifically organized into three main thrusts with many inter-thrust connections, which will increase and strengthen throughout the existence of the Center. We facilitate strong inter-connectivity among all three groups, yielding outstanding scientific synergy for discovery and ideas.

In **Thrust 1** we focus on artificial materials that show functions that emulate the fundamental properties of cells, extracellular matrices, and tissues in the context of energy use and transduction. Our team has identified three primary bio-inspired research areas: artificial muscles, artificial organelles, and stimulusdriven adaptive materials. The work on artificial muscles is focused on systems that can interconvert between chemical and mechanical energy forms (as muscles do). The challenge of discovering the right strategies to transduce stored chemical energy into mechanical motion in materials requires not only synthetic innovation in soft matter but also the use of computational models to find structures in which small energy inputs result in large deformations and forces. In this work, we take advantage of the great computational and theoretical capabilities of the team and also of the enormous recent progress made in DNA nanotechnology to help us discover muscle-like structures in polymer-nucleic acid hybrid materials. Inspired by biological organelles that utilize feedback mechanisms to mediate chemical reactions, we develop artificial organelles that have the capacity to mediate efficiently synthetic reactions as cells do and in ways that chemical laboratories and chemical factories cannot at present. For this purpose, we conduct experiments with precisely positioned micro-particles mediating related chemical events with the goal to discover emergent principles for self-regulating reactions. Another interesting characteristic of biological matter is the ability to dynamically change shape in response to the environment. This characteristic is possibly most prominent in the changes undergone by cells during differentiation, proliferation, and migration, using energy inputs to achieve these functions. In the context of bioinspiration we have defined this problem as the challenge of developing adaptive materials that respond to stimuli such as light and mechanical forces to mutate their structures and properties.

In **Thrust 2** we explore the bottom-up conversion of energy to motion in artificial nanometer to micrometer scale colloids that behave collectively far from equilibrium. Miniaturizing machines down to the nanoscale raises both fundamental questions and novel opportunities to perform tasks that mimic or improve upon biological machines. Unlike most synthetic machines, which rely on centralized engines, biological organisms convert energy into motion in a highly *distributed* fashion: macroscopic forces emerge from the coordinated actions of many chemically powered, molecular scale actuators (motor

proteins). Distributed energy conversion in biology offers several advantages that motivate the pursuit of much simplified non-biological colloidal machines, in which energy is harnessed at colloidal scales to produce emergent behaviors at the mesoscale and perform useful functions at the macroscale. Our work aims to significantly extend these capabilities to create colloidal motors capable of increasingly complex locomotive forms, to control motor activity remotely through external stimuli, to improve the efficiency of colloidal motors by many orders of magnitude, and to engineer switchable interactions among colloidal motors to guide their collective behaviors. By combining computer simulation, continuum modeling, and a suite of experimental systems spanning scales from nano- to macroscopic, the team aims to discover how the distributed activity of ensembles of colloidal motors produce emergent collective behaviors. Once again, cellular behavior inspires our design. Cells undergo dramatic changes in size and shape; they crawl or swim through diverse environments; they capture and transport external cargo; they grow, proliferate, and differentiate; they self-organize to form tissues and organs. Each of these remarkable capabilities relies on the coordinated action of many individual actuators distributed throughout the cell. With this inspiration, the CBES projects aim to create colloidal machines that mimic – in rudimentary form - the mechanical functions of living cells. These non-biological, artificial cells are composed of many colloidal motors within a flexible membrane through which chemical fuel is delivered. Through the collective motions of the confined motors, we envision microscale artificial cells capable of controllable deformations, switchable mechanical properties, and autonomous locomotion. Hierarchical assemblies of these "cells" produce macroscopic, non-equilibrium materials that harness distributed energy conversion and actuation to perform useful functions.

Another critical axis of energy management in biology is connected with modes of charge transport that are not known in artificial matter, such as long-range electron transfer in photosynthesis through media of low conductivity or the selective ionic fluxes across cell membranes that can convert chemical to electrical energy. Therefore in **Thrust 3** we focus sharply on bio-inspired energy and charge transport modes. We are particularly interested in solar energy conversion systems comprising low-dielectric active materials, in which the major obstacle to efficient energy conversion is a low yield of charge collection due to random, rather than directional, motion of electrons. We address this challenge by exploring, computationally and experimentally, the non-equilibrium phenomenon of **quantum ratcheting**. We are also investigating how to control selectivity and directionality of non-equilibrium ion fluxes by theoretically and experimentally designing nanoscale **bio-inspired ion pumps**.

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